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(FILE 'HOME' ENTERED AT 08:17:54 ON 27 SEP 1999)

INDEX 'IMOBILITY, 2MOBILITY, ADISALERTS, AEROSPACE, AGRICOLA,  
AIDSLINE,  
ALUMINIUM, ANABSTR, APILIT, APIPAT, AQUASCI, BIBLIODATA,  
BIOBUSINESS,  
BIOCOMMERCE, BIOSIS, BIOTECHABS, BIOTECHDS, BLLDB, CABA,  
CANCERLIT,  
CAPLUS, CBNB, CEABA, CEN, CERAB, CHEMSAFE, ...' ENTERED AT 08:18:06  
ON 27

SEP 1999

SEA (NMR OR NOESY OR NUCLEAR(W)MAGNETIC(W)RESONANCE)  
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2 FILE AEROSPACE  
106 FILE AGRICOLA  
72 FILE AIDSLINE  
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53 FILE AQUASCI  
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5 FILE SIGLE  
4 FILE SOLIDSTATE  
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342 FILE TOXLINE  
199 FILE TOXLIT  
1024 FILE USPATFULL  
5 FILE WPIDS  
5 FILE WPINDEX  
L1 QUE (NMR OR NOESY OR NUCLEAR(W) MAGNETIC(W)  
RESONANCE) AND (THR  
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FILE 'AGRICOLA, MEDLINE, BIOSIS, CAPLUS, EMBASE, ENERGY, LIFESCI,  
JICST-EPLUS, TOXLINE' ENTERED AT 08:36:39 ON 27 SEP 1999

L2 2072 S L1 AND (FUNCTION OR ACTIVITY)

L3 87 S L2 AND (ALGORITHM#)

L4 40 DUPLICATE REMOVE L3 (47 DUPLICATES REMOVED)

L5 2 S L2 AND (HIGH(W)THROUGHPUT)

=> s l2 and pars?

L6 1 L2 AND PARS?

=> d bib ab

L6 ANSWER 1 OF 1 CAPLUS COPYRIGHT 1999 ACS

AN 1999:146268 CAPLUS

TI \*\*\*Protein\*\*\* \*\*\*NMR\*\*\* and the human proteome project

AU Montelione, Gaetano T.

CS Center for Advanced Biotechnology Medicine and Department of Molecular  
Biology and Biochemistry, Rutgers University, Piscataway, NJ, 08854, USA  
SO Book of Abstracts, 217th ACS National Meeting, Anaheim, Calif., March  
21-25 (1999), POLY-232 Publisher: American Chemical Society, Washington,  
D. C.

CODEN: 67GHA6

DT Conference; Meeting Abstract

LA English

AB Genome sequencing projects are rapidly identifying all of the genes in  
several organisms. The products of these genes are widely recognized as  
the next generation of therapeutics and targets for the development of  
pharmaceuticals. While identification of these genes is proceeding  
quickly, elucidation of their \*\*\*three\*\*\* \*\*\*dimensional\*\*\* (3D)  
structures and biochem. functions lags far behind. In some cases,  
knowledge of 3D structures of \*\*\*proteins\*\*\* can provide important  
insights into structural homol. that is not easily recognized by sequence  
alignment comparisons. Thus, anal. of a \*\*\*protein\*\*\* 's 3D structure  
by \*\*\*NMR\*\*\* or X-ray crystallog. prior to characterization of the  
\*\*\*protein\*\*\* 's biochem. \*\*\*function\*\*\* can sometimes provide key  
information regarding \*\*\*protein\*\*\* fold class, locations and  
clustering of conserved residues, and surface electrostatic field  
distributions. This information can be used to develop hypotheses  
regarding potential biochem. functions, and the resulting limited set of  
putative biochem. functions tested by appropriate biochem. assays.  
\*\*\*NMR\*\*\* chem. shift assignments and soln. structures of  
\*\*\*proteins\*\*\* also provide the basis for epitope-mapping, mol.  
dynamics, and SAR studies, and set the stage for subsequent drug  
development using combinatorial and/or rational design methods. We are  
developing technologies that will significantly accelerate the process of  
structure detn. by \*\*\*NMR\*\*\*. These include bioinformatics methods  
for \*\*\*parsing\*\*\* novel genes into domain encoding regions, high-level  
"multiplexed" \*\*\*protein\*\*\* expression systems, and \*\*\*NMR\*\*\*  
pulse sequences, data collection methods, and expert-system software for  
automated anal. of \*\*\*protein\*\*\* resonance assignments and 3D  
structures. These technologies and the resulting exptl. data are being  
organized and integrated using relational databases. The goal of this  
work is to develop a "high-throughput" process for structural anal. of  
novel gene products on a genomic scale. In a pilot project, these  
techniques are being applied to clusters of orthologous genes coding for  
\*\*\*proteins\*\*\* of unknown structure and \*\*\*function\*\*\*, with the aim  
of testing the hypothesis that 3D structural anal. can sometimes provide  
useful and important clues regarding the biochem. functions of orphan gene  
products. The relationship of our effort and the emerging international  
interest in a large-scale Human Proteome Project will be discussed.

=> s l2 and multiplex?

L7 1 L2 AND MULTIPLEX?

=> s l2 and (structure# (4a) function?)

6 FILES SEARCHED...

L8 428 L2 AND (STRUCTURE# (4A) FUNCTION?)

=> duplicate remove l8

DUPLICATE PREFERENCE IS 'AGRICOLA, MEDLINE, BIOSIS, CAPLUS,  
EMBASE, ENERGY, LIFESCI, JICST-EPLUS, TOXLINE'  
KEEP DUPLICATES FROM MORE THAN ONE FILE? Y/(N):n

PROCESSING COMPLETED FOR L8

L9 189 DUPLICATE REMOVE L8 (239 DUPLICATES REMOVED)

=> d 1-189 ti

L9 ANSWER 1 OF 189 CAPLUS COPYRIGHT 1999 ACS

TI Compositions and methods to inhibit formation of the C5B-9 complex of  
complement

L9 ANSWER 2 OF 189 CAPLUS COPYRIGHT 1999 ACS

TI Linking gene sequence to gene \*\*\*function\*\*\* by \*\*\*three\*\*\* -  
\*\*\*dimensional\*\*\* \*\*\*protein\*\*\* \*\*\*structure\*\*\* determination  
using \*\*\*NMR\*\*\*

L9 ANSWER 3 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS

T1 The AcbC \*\*\*protein\*\*\* from *Actinoplanes* species is a C7-cyclitol synthase related to 3-dehydroquinate synthases and is involved in the biosynthesis of the alpha-glucosidase inhibitor acarbose.

L9 ANSWER 4 OF 189 MEDLINE

T1 Effects of substitutions of lysine and aspartic acid for asparagine at beta 108 and of tryptophan for valine at alpha 96 on the structural and functional properties of human normal adult hemoglobin: roles of alpha 1 beta 1 and alpha 1 beta 2 subunit interfaces in the cooperative oxygenation process.

L9 ANSWER 5 OF 189 MEDLINE

DUPLICATE 1

T1 \*\*\*NMR\*\*\* \*\*\*structure\*\*\* and \*\*\*functional\*\*\* studies of the Mu repressor DNA-binding domain.

L9 ANSWER 6 OF 189 MEDLINE

DUPLICATE 2

T1 Disulfide bridges in interleukin-8 probed using non-natural disulfide analogues: dissociation of roles in \*\*\*structure\*\*\* from \*\*\*function\*\*\*.

L9 ANSWER 7 OF 189 MEDLINE

DUPLICATE 3

T1 Solution structure of the chicken cysteine-rich \*\*\*protein\*\*\*, CRP1, a double-LIM \*\*\*protein\*\*\* implicated in muscle differentiation.

L9 ANSWER 8 OF 189 MEDLINE

DUPLICATE 4

T1 Structure and dynamics of \*\*\*peptide\*\*\*-amphiphiles incorporating triple-helical proteinlike molecular architecture.

L9 ANSWER 9 OF 189 CAPLUS COPYRIGHT 1999 ACS

DUPLICATE 5

T1 Comparative modeling of amoebapores and granulysin based on the NK-lysin \*\*\*structure\*\*\*. Structural and \*\*\*functional\*\*\* implications

L9 ANSWER 10 OF 189 CAPLUS COPYRIGHT 1999 ACS

DUPLICATE 6

T1 Autoprocessing of HIV-1 protease is tightly coupled to \*\*\*protein\*\*\* folding

L9 ANSWER 11 OF 189 MEDLINE

DUPLICATE 7

T1 The solution structure of a superpotent B-chain-shortened single-replacement insulin analogue.

L9 ANSWER 12 OF 189 MEDLINE

DUPLICATE 8

T1 Solution structure of toxin 2 from centruroides noxius Hoffmann, a beta-scorpion neurotoxin acting on sodium channels.

L9 ANSWER 13 OF 189 MEDLINE

DUPLICATE 9

T1 Chimeras of human extracellular and intracellular superoxide dismutases. Analysis of \*\*\*structure\*\*\* and \*\*\*function\*\*\* of the individual domains.

L9 ANSWER 14 OF 189 ENERGY COPYRIGHT 1999 USDOE/IEA-ETDE

T1 Effective computational strategies for determining structures of carcinogen-damaged DNA.

L9 ANSWER 15 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS

T1 Motional dynamics of the catalytic loop in OMP synthase.

L9 ANSWER 16 OF 189 MEDLINE

DUPLICATE 10

T1 Smoluchowski dynamics of the vnd/NK-2 homeodomain from *Drosophila melanogaster*: first-order mode-coupling approximation.

L9 ANSWER 17 OF 189 CAPLUS COPYRIGHT 1999 ACS

T1 \*\*\*Protein\*\*\* \*\*\*NMR\*\*\* and the human proteome project

L9 ANSWER 18 OF 189 MEDLINE

DUPLICATE 11

T1 Secondary structure of the C-terminal DNA-binding domain of the transcriptional activator NifA from *Klebsiella pneumoniae*: spectroscopic analyses.

L9 ANSWER 19 OF 189 MEDLINE

DUPLICATE 12

T1 Purification and characterization of a plant antimicrobial \*\*\*peptide\*\*\* expressed in *Escherichia coli*.

L9 ANSWER 20 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS

T1 Characterization of \*\*\*protein\*\*\*-glycolipid recognition at the membrane bilayer.

L9 ANSWER 21 OF 189 CAPLUS COPYRIGHT 1999 ACS

DUPLICATE 13

T1 Acylation-stimulating \*\*\*protein\*\*\* (ASP): \*\*\*structure\*\*\* - \*\*\*function\*\*\* determinants of cell surface binding and triacylglycerol synthetic \*\*\*activity\*\*\*

L9 ANSWER 22 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS

T1 Structural biology of HIV.

L9 ANSWER 23 OF 189 TOXLINE

T1 MUTAGENESIS AND REPAIR OF DNA.

L9 ANSWER 24 OF 189 TOXLINE

T1 ISOTOPIC PROBES OF ENZYMATIC REACTION MECHANISMS.

L9 ANSWER 25 OF 189 CAPLUS COPYRIGHT 1999 ACS

T1 Characterization of antibacterial COOH-terminal proenkephalin-A-derived \*\*\*peptides\*\*\* (PEAP) in infectious fluids. Importance of enkephalin, the antibacterial PEAP209-237 secreted by stimulated chromaffin cells

L9 ANSWER 26 OF 189 MEDLINE

DUPLICATE 14

T1 Yeast transcript elongation factor (TFIIS), \*\*\*structure\*\*\* and \*\*\*function\*\*\*. I: \*\*\*NMR\*\*\* structural analysis of the minimal transcriptionally active region.

L9 ANSWER 27 OF 189 MEDLINE

DUPLICATE 15

T1 High-resolution solution \*\*\*NMR\*\*\* structure of the minimal active domain of the human immunodeficiency virus type-2 nucleocapsid \*\*\*protein\*\*\*.

L9 ANSWER 28 OF 189 EMBASE COPYRIGHT 1999 ELSEVIER SCI. B. V.

T1 Functional requirements for specific ligand recognition by a biotin-binding rna pseudoknot.

L9 ANSWER 29 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS

T1 The \*\*\*NMR\*\*\* structure of *Escherichia coli* ribosomal \*\*\*protein\*\*\* L25 shows homology to general stress \*\*\*proteins\*\*\* and glutamyl-tRNA synthetases.

L9 ANSWER 30 OF 189 EMBASE COPYRIGHT 1999 ELSEVIER SCI. B. V.

T1 Conformational analysis and automated receptor docking of selective arylacetamide-based .kappa.-opioid agonists.

L9 ANSWER 31 OF 189 AGRICOLA

DUPLICATE 16

T1 Micelle stability: kappa-casein \*\*\*structure\*\*\* and \*\*\*function\*\*\*

L9 ANSWER 32 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS

T1 Solution structure of the SH3 domain from Bruton's tyrosine kinase.

L9 ANSWER 33 OF 189 CAPLUS COPYRIGHT 1999 ACS

T1 Structure of human cyclin-dependent kinase inhibitor p19INK4d: comparison to known ankyrin-repeat-containing structures and implications for the dysfunction of tumor suppressor p16INK4a

L9 ANSWER 34 OF 189 MEDLINE

DUPLICATE 17

T1 Method for prediction of \*\*\*protein\*\*\* \*\*\*function\*\*\* from sequence using the sequence-to- \*\*\*structure\*\*\* -to- \*\*\*function\*\*\* paradigm with application to glutaredoxins/thioredoxins and T1 ribonucleases.

L9 ANSWER 35 OF 189 EMBASE COPYRIGHT 1999 ELSEVIER SCI. B. V.

T1 Solution structure of Compstatin, a potent complement inhibitor.

L9 ANSWER 36 OF 189 MEDLINE

DUPLICATE 18

T1 The relationship between insulin bioactivity and structure in the NH2-terminal A-chain helix.

L9 ANSWER 37 OF 189 MEDLINE

T1 Recent trends in \*\*\*protein\*\*\* structural studies.

L9 ANSWER 38 OF 189 MEDLINE

DUPLICATE 19

T1 \*\*\*Structure\*\*\* - \*\*\*function\*\*\* analysis of a series of glucagon-like \*\*\*peptide\*\*\* -1 analogs.

L9 ANSWER 39 OF 189 MEDLINE

DUPLICATE 20

T1 The \*\*\*structure\*\*\* and \*\*\*function\*\*\* of HPr.

L9 ANSWER 40 OF 189 CAPLUS COPYRIGHT 1999 ACS

T1 The development of \*\*\*NMR\*\*\* methods to study \*\*\*protein\*\*\* structure and dynamics

L9 ANSWER 41 OF 189 MEDLINE

DUPLICATE 21

T1 Non-homology knowledge-based prediction of the papain prosegment folding pattern: a description of plausible folding and activation mechanisms.

L9 ANSWER 42 OF 189 EMBASE COPYRIGHT 1999 ELSEVIER SCI. B. V.

T1 Probing the structure of the human Ca2+- and Zn2+-binding \*\*\*protein\*\*\* S100A3: Spectroscopic investigations of its transition metal ion complexes, and \*\*\*three\*\*\* - \*\*\*dimensional\*\*\* structural model.

L9 ANSWER 43 OF 189 MEDLINE

DUPLICATE 22

T1 Energy strain in \*\*\*three\*\*\* - \*\*\*dimensional\*\*\* \*\*\*protein\*\*\* structures.

L9 ANSWER 44 OF 189 EMBASE COPYRIGHT 1999 ELSEVIER SCI. B. V.

T1 The atypical serine proteases of the complement system.

L9 ANSWER 45 OF 189 MEDLINE

DUPLICATE 23

T1 \*\*\*Structure\*\*\* - \*\*\*function\*\*\* relationships of antimicrobial \*\*\*peptides\*\*\*.

L9 ANSWER 46 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS

T1 \*\*\*NMR\*\*\* analysis of a potent decapeptide agonist of human C5a anaphylatoxin.

L9 ANSWER 47 OF 189 MEDLINE DUPLICATE 24  
T1 Sequence-specific 1H assignment and secondary structure of the bacteriocin AS-48 cyclic \*\*\*peptide\*\*\*.

L9 ANSWER 48 OF 189 MEDLINE DUPLICATE 25  
T1 Structure and properties of surfactant \*\*\*protein\*\*\* C.

L9 ANSWER 49 OF 189 JICST-EPLUS COPYRIGHT 1999 JST  
T1 \*\*\*Three\*\*\* . \*\*\*dimensional\*\*\* Structure of DELTA-conotoxin TxVIA.

L9 ANSWER 50 OF 189 CAPLUS COPYRIGHT 1999 ACS  
T1 Insights into the structure of hepatocyte growth factor/scatter factor (HGF/SF) and implications for receptor activation

L9 ANSWER 51 OF 189 MEDLINE DUPLICATE 26  
T1 Mini-proinsulin and mini-IGF-I: homologous \*\*\*protein\*\*\* sequences encoding non-homologous structures.

L9 ANSWER 52 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS DUPLICATE 27  
T1 \*\*\*Structure\*\*\* and \*\*\*function\*\*\* of \*\*\*peptide\*\*\* and \*\*\*protein\*\*\* toxins from marine organisms.

L9 ANSWER 53 OF 189 EMBASE COPYRIGHT 1999 ELSEVIER SCI. B.V.  
T1 Metal coordination of azurin in the unfolded state.

L9 ANSWER 54 OF 189 EMBASE COPYRIGHT 1999 ELSEVIER SCI. B.V.  
T1 Accessibility of selenomethionine \*\*\*proteins\*\*\* by total chemical synthesis: Structural studies of human herpesvirus-8 MIP-II.

L9 ANSWER 55 OF 189 CAPLUS COPYRIGHT 1999 ACS  
T1 \*\*\*Structure\*\*\* and \*\*\*function\*\*\* of charybdotoxin are not affected by substitution of an interior cysteine with two alpha-amino-n-butyric acid (Aba) residues

L9 ANSWER 56 OF 189 CAPLUS COPYRIGHT 1999 ACS DUPLICATE 28  
T1 The role of leucine residues in the \*\*\*structure\*\*\* and \*\*\*function\*\*\* of a leucine zipper \*\*\*peptide\*\*\* inhibitor of paramyxovirus (NDV) fusion

L9 ANSWER 57 OF 189 CAPLUS COPYRIGHT 1999 ACS  
T1 Synthetic RNA modification and crosslinking approaches towards the structure of the hairpin ribozyme and the HIV-1 Tat \*\*\*protein\*\*\* interaction with TAR RNA

L9 ANSWER 58 OF 189 JICST-EPLUS COPYRIGHT 1999 JST  
T1 Modern \*\*\*NMR\*\*\* Spectroscopy and X-ray Crystallography: a different approach to study the \*\*\*structure\*\*\* and its \*\*\*function\*\*\* of a \*\*\*protein\*\*\*.

L9 ANSWER 59 OF 189 EMBASE COPYRIGHT 1999 ELSEVIER SCI. B.V.  
T1 \*\*\*Three\*\*\* . \*\*\*dimensional\*\*\* \*\*\*structure\*\*\* of lactoferrin: Implications for \*\*\*function\*\*\*, including comparisons with transferrin.

L9 ANSWER 60 OF 189 TOXLINE  
T1 MUTAGENESIS AND REPAIR OF DNA.

L9 ANSWER 61 OF 189 TOXLINE  
T1 ISOTOPIC PROBES OF ENZYMATIC REACTION MECHANISMS.

L9 ANSWER 62 OF 189 MEDLINE DUPLICATE 29  
T1 Site-directed mutagenesis and characterization of uracil-DNA glycosylase inhibitor \*\*\*protein\*\*\*. Role of specific carboxylic amino acids in complex formation with Escherichia coli uracil-DNA glycosylase.

L9 ANSWER 63 OF 189 MEDLINE DUPLICATE 30  
T1 Comparison of the hemolytic \*\*\*activity\*\*\* and solution structures of two snake venom cardiotoxin analogues which only differ in their N-terminal amino acid.

L9 ANSWER 64 OF 189 LIFESCI COPYRIGHT 1999 CSA  
T1 Comparison of the hemolytic \*\*\*activity\*\*\* and solution structures of two snake venom cardiotoxin analogues which only differ in their N-terminal amino acid

L9 ANSWER 65 OF 189 MEDLINE DUPLICATE 31  
T1 Structural mimicry of a native \*\*\*protein\*\*\* by a minimized binding domain.

L9 ANSWER 66 OF 189 MEDLINE DUPLICATE 32  
T1 Structure of the C-terminal fragment 300-320 of the rat angiotensin II AT1A receptor and its relevance with respect to G- \*\*\*protein\*\*\* coupling.

L9 ANSWER 67 OF 189 CAPLUS COPYRIGHT 1999 ACS DUPLICATE 33  
T1 \*\*\*Structure\*\*\* and \*\*\*Function\*\*\* of an Aromatic Ensemble That

Restricts the Dynamics of the Hydrophobic Core of a Designed Helix-Loop-Helix Dimer

L9 ANSWER 68 OF 189 MEDLINE DUPLICATE 34  
T1 Solution structure of the Mu end DNA-binding beta subdomain of phage Mu transposase: modular DNA recognition by two tethered domains.

L9 ANSWER 69 OF 189 MEDLINE DUPLICATE 35  
T1 Solution \*\*\*structure\*\*\* and basis for \*\*\*functional\*\*\* \*\*\*activity\*\*\* of stromal cell-derived factor-1; dissociation of CXCR4 activation from binding and inhibition of HIV-1.

L9 ANSWER 70 OF 189 CAPLUS COPYRIGHT 1999 ACS  
T1 On the convergent evolution of animal toxins. Conservation of a diad of functional residues in potassium channel-blocking toxins with unrelated structures

L9 ANSWER 71 OF 189 MEDLINE DUPLICATE 36  
T1 TESS: a geometric hashing algorithm for deriving 3D coordinate templates for searching structural databases. Application to enzyme active sites.

L9 ANSWER 72 OF 189 CAPLUS COPYRIGHT 1999 ACS  
T1 Cloning, purification, and preliminary characterization by circular dichroism and \*\*\*NMR\*\*\* of a carboxyl-terminal domain of the bacteriophage P22 scaffolding \*\*\*protein\*\*\*

L9 ANSWER 73 OF 189 MEDLINE DUPLICATE 37  
T1 \*\*\*Structure\*\*\* . \*\*\*function\*\*\* relationships of cellular retinoic acid-binding \*\*\*proteins\*\*\*. Quantitative analysis of the ligand binding properties of the wild-type \*\*\*proteins\*\*\* and site-directed mutants.

L9 ANSWER 74 OF 189 MEDLINE DUPLICATE 38  
T1 Assessment by 1H \*\*\*NMR\*\*\* spectroscopy of the structural behaviour of human parathyroid-hormone-related \*\*\*protein\*\*\* (1-34) and its close relationship with the N-terminal fragments of human parathyroid hormone in solution.

L9 ANSWER 75 OF 189 EMBASE COPYRIGHT 1999 ELSEVIER SCI. B.V.  
T1 The collagen triple-helix structure.

L9 ANSWER 76 OF 189 EMBASE COPYRIGHT 1999 ELSEVIER SCI. B.V.  
T1 Snake venom cardiotoxins- \*\*\*structure\*\*\*, dynamics, \*\*\*function\*\*\* and folding.

L9 ANSWER 77 OF 189 MEDLINE DUPLICATE 39  
T1 The second Kunitz domain of human tissue factor pathway inhibitor: cloning, structure determination and interaction with factor Xa.

L9 ANSWER 78 OF 189 MEDLINE DUPLICATE 40  
T1 Refined solution structure of the anti-mammal and anti-insect LqIII scorpion toxin: comparison with other scorpion toxins.

L9 ANSWER 79 OF 189 MEDLINE DUPLICATE 41  
T1 Solution structure of a type 2 module from fibronectin: implications for the \*\*\*structure\*\*\* and \*\*\*function\*\*\* of the gelatin-binding domain.

L9 ANSWER 80 OF 189 MEDLINE DUPLICATE 42  
T1 The pH-dependent \*\*\*tertiary\*\*\* \*\*\*structure\*\*\* of a designed helix-loop-helix dimer.

L9 ANSWER 81 OF 189 MEDLINE DUPLICATE 43  
T1 Analysis of a \*\*\*peptide\*\*\* inhibitor of paramyxovirus (NDV) fusion using biological assays, \*\*\*NMR\*\*\*, and molecular modeling.

L9 ANSWER 82 OF 189 AGRICOLA DUPLICATE 44  
T1 Solution structure of Lqh-8/6, a toxin-like \*\*\*peptide\*\*\* from a scorpion venom. Structural heterogeneity induced by proline cis/trans isomerization.

L9 ANSWER 83 OF 189 LIFESCI COPYRIGHT 1999 CSA  
T1 Higher order structures of coxsackievirus B 5' nontranslated region RNA

L9 ANSWER 84 OF 189 CAPLUS COPYRIGHT 1999 ACS  
T1 Amylin, calcitonin gene-related \*\*\*peptide\*\*\*, calcitonin, and adrenomedullin: a \*\*\*peptide\*\*\* superfamily

L9 ANSWER 85 OF 189 MEDLINE  
T1 Endo-beta-1,4-xylanase families: differences in catalytic properties.

L9 ANSWER 86 OF 189 CAPLUS COPYRIGHT 1999 ACS  
T1 \*\*\*Three\*\*\* . \*\*\*dimensional\*\*\* structure and receptor-recognition sites of bombyxin-II, an insulin-like brain-secretory \*\*\*peptide\*\*\* of the silkworm

L9 ANSWER 87 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS  
T1 Alterations in chemical shifts and exchange broadening upon \*\*\*peptide\*\*\* boronic acid inhibitor binding to alpha-lytic protease.

- L9 ANSWER 88 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS  
T1 \*\*\*NMR\*\*\* -based \*\*\*structure\*\*\* . \*\*\*function\*\*\* relation of N-type inactivation in K-v-type K<sup>+</sup> channels.
- L9 ANSWER 89 OF 189 AGRICOLA DUPLICATE 45  
T1 \*\*\*NMR\*\*\* methods for the study of \*\*\*protein\*\*\* structure and dynamics.
- L9 ANSWER 90 OF 189 AGRICOLA DUPLICATE 46  
T1 1H \*\*\*NMR\*\*\* assignment and global fold of napin Bn1b, a representative 2S albumin seed \*\*\*protein\*\*\* .
- L9 ANSWER 91 OF 189 MEDLINE DUPLICATE 47  
T1 \*\*\*Three\*\*\* . \*\*\*dimensional\*\*\* solution structure of mu-conotoxin GIIB, a specific blocker of skeletal muscle sodium channels.
- L9 ANSWER 92 OF 189 MEDLINE DUPLICATE 48  
T1 The cytoplasmic fragment of the aspartate receptor displays globally dynamic behavior.
- L9 ANSWER 93 OF 189 MEDLINE DUPLICATE 49  
T1 Circularly permuted dihydrofolate reductase possesses all the properties of the molten globule state, but can resume \*\*\*functional\*\*\* sites of \*\*\*tertiary\*\*\* \*\*\*structure\*\*\* by interaction with its ligands.
- L9 ANSWER 94 OF 189 CAPLUS COPYRIGHT 1999 ACS DUPLICATE 50  
T1 \*\*\*Tertiary\*\*\* \*\*\*structure\*\*\* and \*\*\*functional\*\*\* sites of bombyxin, an insect insulin-like \*\*\*peptide\*\*\* . Comparison with those of insulin
- L9 ANSWER 95 OF 189 MEDLINE DUPLICATE 51  
T1 1H and 15N \*\*\*nuclear\*\*\* \*\*\*magnetic\*\*\* \*\*\*resonance\*\*\* assignment and secondary structure of the cytotoxic ribonuclease alpha-Sarcin.
- L9 ANSWER 96 OF 189 MEDLINE DUPLICATE 52  
T1 What \*\*\*function\*\*\* for human lithostathine?: structural investigations by \*\*\*three\*\*\* . \*\*\*dimensional\*\*\* structure modeling and high-resolution \*\*\*NMR\*\*\* spectroscopy.
- L9 ANSWER 97 OF 189 MEDLINE DUPLICATE 53  
T1 Computer modeling of 3D structures of cytochrome P450s.
- L9 ANSWER 98 OF 189 CAPLUS COPYRIGHT 1999 ACS  
T1 \*\*\*Structure\*\*\* . \*\*\*function\*\*\* relationship of adenylate kinase: Glu-101 in AMP specificity
- L9 ANSWER 99 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS  
T1 Solution structure of protegrin-1, a broad-spectrum antimicrobial \*\*\*peptide\*\*\* from porcine leukocytes.
- L9 ANSWER 100 OF 189 MEDLINE  
T1 Domain organizations of modular extracellular matrix \*\*\*proteins\*\*\* and their evolution.
- L9 ANSWER 101 OF 189 MEDLINE DUPLICATE 54  
T1 \*\*\*Structure\*\*\* . \*\*\*function\*\*\* relationships of the complement regulatory \*\*\*protein\*\*\*, CD59.
- L9 ANSWER 102 OF 189 MEDLINE  
T1 Synthesis and conformational analysis by 1H \*\*\*NMR\*\*\* and restrained molecular dynamics simulations of the cyclic decapeptide [Ser-Tyr-Ser-Met-Glu-His-Phe-Arg-Trp-Gly].
- L9 ANSWER 103 OF 189 CAPLUS COPYRIGHT 1999 ACS  
T1 High frequency of mutational changes during the cloning of a human centromeric repeat
- L9 ANSWER 104 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS  
T1 \*\*\*NMR\*\*\* structure of HM1B from the hyperthermophile, Methanothermus fervidus, confirms that this archaeal \*\*\*protein\*\*\* is a histone.
- L9 ANSWER 105 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS DUPLICATE 55  
T1 3-D Reconstructions from ice-embedded and negatively stained biomacromolecular assemblies: A critical comparison.
- L9 ANSWER 106 OF 189 CAPLUS COPYRIGHT 1999 ACS DUPLICATE 56  
T1 Modern \*\*\*NMR\*\*\* spectroscopy and x-ray crystallography. Different approaches to study the \*\*\*structure\*\*\* and its \*\*\*function\*\*\* of a \*\*\*protein\*\*\*
- L9 ANSWER 107 OF 189 CAPLUS COPYRIGHT 1999 ACS  
T1 Structure of a cyclic \*\*\*peptide\*\*\* with a catalytic triad, determined by computer simulation and \*\*\*NMR\*\*\* spectroscopy
- L9 ANSWER 108 OF 189 CAPLUS COPYRIGHT 1999 ACS  
T1 \*\*\*Structure\*\*\* and \*\*\*function\*\*\* of the single-stranded DNA binding \*\*\*proteins\*\*\* of the filamentous bacteriophages M13 and Pf3. \*\*\*NMR\*\*\* studies
- L9 ANSWER 109 OF 189 TOXLINE  
T1 BIOLOGICAL CONSEQUENCES OF SITE-SPECIFIC DAMAGE TO DNA.
- L9 ANSWER 110 OF 189 CAPLUS COPYRIGHT 1999 ACS  
T1 Reactive-Site Hydrolyzed Cucurbita maxima Trypsin Inhibitor-V: \*\*\*Function\*\*\*, Thermodynamic Stability, and \*\*\*NMR\*\*\* Solution Structure
- L9 ANSWER 111 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS  
T1 Catalytic domain of human immunodeficiency virus type 1 integrase: Identification of a soluble mutant by systematic replacement of hydrophobic residues.
- L9 ANSWER 112 OF 189 MEDLINE DUPLICATE 57  
T1 Biological and structural characterization of a Ras transforming mutation at the phenylalanine-156 residue, which is conserved in all members of the Ras superfamily.
- L9 ANSWER 113 OF 189 MEDLINE DUPLICATE 58  
T1 The zinc coordination site of the bacteriophage Mu translational activator \*\*\*protein\*\*\*, Com.
- L9 ANSWER 114 OF 189 MEDLINE DUPLICATE 59  
T1 \*\*\*Structure\*\*\* . \*\*\*function\*\*\* studies of mEGF: probing the type I beta-turn between residues 25 and 26.
- L9 ANSWER 115 OF 189 CAPLUS COPYRIGHT 1999 ACS  
T1 Determination of the structure of exochelin MN, the extracellular siderophore from Mycobacterium neoaurum
- L9 ANSWER 116 OF 189 MEDLINE DUPLICATE 60  
T1 Structures of bacterial immunoglobulin-binding domains and their complexes with immunoglobulins.
- L9 ANSWER 117 OF 189 CAPLUS COPYRIGHT 1999 ACS  
T1 Determination of the solution structure of apo calbindin D9k by \*\*\*NMR\*\*\* spectroscopy
- L9 ANSWER 118 OF 189 CAPLUS COPYRIGHT 1999 ACS  
T1 \*\*\*Three\*\*\* \*\*\*dimensional\*\*\* structure of .omega.-agatoxin IVA determined by 1H- \*\*\*NMR\*\*\*
- L9 ANSWER 119 OF 189 CAPLUS COPYRIGHT 1999 ACS  
T1 Mass spectrometric approaches to the characterization of tertiary and supramolecular structures of biomacromolecules
- L9 ANSWER 120 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS  
T1 \*\*\*NMR\*\*\*: This other method for \*\*\*protein\*\*\* and nucleic acid structure determination.
- L9 ANSWER 121 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS  
T1 Water molecules within and around \*\*\*proteins\*\*\*
- L9 ANSWER 122 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS  
T1 Solution structure of the DNA binding domain of a nucleoid-associated \*\*\*protein\*\*\*, H-NS, from Escherichia coli.
- L9 ANSWER 123 OF 189 MEDLINE DUPLICATE 61  
T1 Solution \*\*\*structure\*\*\* and \*\*\*function\*\*\* in trifluoroethanol of PP-50, an ATP-binding \*\*\*peptide\*\*\* from FIATPase.
- L9 ANSWER 124 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS  
T1 Structure of the presynaptic (Y-2) receptor-specific neuropeptide Y analog ANA-NPY.
- L9 ANSWER 125 OF 189 CAPLUS COPYRIGHT 1999 ACS DUPLICATE 62  
T1 \*\*\*Structure\*\*\* and \*\*\*function\*\*\* of \*\*\*protein\*\*\* modules
- L9 ANSWER 126 OF 189 MEDLINE DUPLICATE 63  
T1 \*\*\*Three\*\*\* . \*\*\*dimensional\*\*\* structures of alpha and beta chemokines.
- L9 ANSWER 127 OF 189 ENERGY COPYRIGHT 1999 USDOE/IEA-ETDE  
T1 Structural studies on leukaemia inhibitory factor.
- L9 ANSWER 128 OF 189 TOXLINE  
T1 BIOLOGICAL CONSEQUENCES OF SITE-SPECIFIC DAMAGE TO DNA.
- L9 ANSWER 129 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS  
T1 \*\*\*Function\*\*\* and \*\*\*three\*\*\* . \*\*\*dimensional\*\*\* \*\*\*structure\*\*\* of \*\*\*proteins\*\*\* using \*\*\*nuclear\*\*\* \*\*\*magnetic\*\*\* \*\*\*resonance\*\*\* spectroscopy.
- L9 ANSWER 130 OF 189 EMBASE COPYRIGHT 1999 ELSEVIER SCI. B.V.  
T1 Sialyl Lewis X mimics derived from a pharmacophore search are selectin inhibitors with anti-inflammatory \*\*\*activity\*\*\*
- L9 ANSWER 131 OF 189 MEDLINE DUPLICATE 64  
T1 Receptor-binding affinities of human epidermal growth factor variants

having unnatural amino acid residues in position 23.

L9 ANSWER 132 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS

T1 DNA binding and bending properties of the post-meiotically expressed Sry-related \*\*\*protein\*\*\* Sox-5.

L9 ANSWER 133 OF 189 MEDLINE DUPLICATE 65

T1 Site-directed mutagenesis in hemoglobin: functional and structural role of the penultimate tyrosine in the alpha subunit.

L9 ANSWER 134 OF 189 CAPLUS COPYRIGHT 1999 ACS

T1 \*\*\*Three\*\*\* \*\*\*dimensional\*\*\* structures of SH2 and SH3 domains

L9 ANSWER 135 OF 189 MEDLINE

T1 Cardiotoxin III from the Taiwan cobra (Naja naja atra). Determination of structure in solution and comparison with short neurotoxins.

L9 ANSWER 136 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS

T1 Solution structure of a specific DNA complex of the Myb DNA-binding domain with cooperative recognition helices.

L9 ANSWER 137 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS

T1 Solution structure of a gamma-carboxyglutamic acid-rich \*\*\*peptide\*\*\* of factor IX by two-dimensional \*\*\*nuclear\*\*\* \*\*\*magnetic\*\*\* \*\*\*resonance\*\*\* spectroscopy.

L9 ANSWER 138 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS

T1 Solution structure of a cysteine rich domain of rat \*\*\*protein\*\*\* kinase C.

L9 ANSWER 139 OF 189 MEDLINE

T1 Empirical studies of \*\*\*protein\*\*\* secondary structure by vibrational circular dichroism and related techniques. Alpha-lactalbumin and lysozyme as examples.

L9 ANSWER 140 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS

T1 Stabilized \*\*\*NMR\*\*\* structure of the hypercalcemia of malignancy \*\*\*peptide\*\*\* PTHrP(Ala-26)(1-34) amide.

L9 ANSWER 141 OF 189 CAPLUS COPYRIGHT 1999 ACS

T1 Structure of the C3HC4 domain by 1H- \*\*\*nuclear\*\*\* \*\*\*magnetic\*\*\* \*\*\*resonance\*\*\* spectroscopy. A new structural class of zinc-finger

L9 ANSWER 142 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS

T1 Structure of a soluble, glycosylated form of the human complement regulatory \*\*\*protein\*\*\* CD59.

L9 ANSWER 143 OF 189 EMBASE COPYRIGHT 1999 ELSEVIER SCI. B.V.

T1 \*\*\*Structure\*\*\* and \*\*\*function\*\*\* of IRES, the noncoding mRNA sequences regulating synthesis of ferritin, transferrin receptor and (erythroid) 5- aminolevulinate synthase.

L9 ANSWER 144 OF 189 MEDLINE DUPLICATE 66

T1 \*\*\*Structure\*\*\* - \*\*\*function\*\*\* studies of [2Fe-2S] ferredoxins.

L9 ANSWER 145 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS

T1 Structure and dynamics of the neutrophil defensins NP-2, NP-5, and HNP-1: \*\*\*NMR\*\*\* studies of amide hydrogen exchange kinetics.

L9 ANSWER 146 OF 189 CAPLUS COPYRIGHT 1999 ACS

T1 Solution structure of RP 71955, a new 21 amino acid tricyclic \*\*\*peptide\*\*\* active against HIV-1 virus

L9 ANSWER 147 OF 189 CAPLUS COPYRIGHT 1999 ACS

T1 \*\*\*Function\*\*\* and \*\*\*three\*\*\* - \*\*\*dimensional\*\*\* \*\*\*structure\*\*\* of \*\*\*proteins\*\*\* using \*\*\*nuclear\*\*\* \*\*\*magnetic\*\*\* \*\*\*resonance\*\*\* spectroscopy

L9 ANSWER 148 OF 189 MEDLINE DUPLICATE 67

T1 Primary and \*\*\*three\*\*\* - \*\*\*dimensional\*\*\* structure of lactotransferrin (lactoferrin) glycans

L9 ANSWER 149 OF 189 TOXLINE

T1 \*\*\*STRUCTURE\*\*\* - \*\*\*FUNCTION\*\*\* STUDY OF COBRATOXIN.

L9 ANSWER 150 OF 189 MEDLINE DUPLICATE 68

T1 Solution structure of a complex between [N-MeCys3,N-MeCys7]TANDEM and [d(GATATC)]2.

L9 ANSWER 151 OF 189 MEDLINE DUPLICATE 69

T1 The role of asparagine-32 in forming the receptor-binding epitope of human epidermal growth factor.

L9 ANSWER 152 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS DUPLICATE 70

T1 The use of osmolytes to facilitate \*\*\*protein\*\*\* \*\*\*NMR\*\*\* spectroscopy.

L9 ANSWER 153 OF 189 MEDLINE

T1 \*\*\*Structure\*\*\* and \*\*\*function\*\*\* of phosphatidylinositol 3-kinase: a potential second messenger system involved in growth control.

L9 ANSWER 154 OF 189 MEDLINE DUPLICATE 71

T1 An automated method for modeling \*\*\*proteins\*\*\* on known templates using distance geometry.

L9 ANSWER 155 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS

T1 The use of synthetic \*\*\*peptides\*\*\* to unravel the mechanism of muscle regulation.

L9 ANSWER 156 OF 189 CAPLUS COPYRIGHT 1999 ACS

T1 Folding topology and DNA binding of the N-terminal fragment of Ada \*\*\*protein\*\*\*

L9 ANSWER 157 OF 189 TOXLINE

T1 CHEMICAL/IMMUNOCHEMICAL STUDIES OF MYOTOXIC \*\*\*PROTEINS\*\*\*

L9 ANSWER 158 OF 189 TOXLINE

T1 \*\*\*STRUCTURE\*\*\* - \*\*\*FUNCTION\*\*\* STUDIES ON MICROSOMAL MEMBRANES.

L9 ANSWER 159 OF 189 MEDLINE

DUPLICATE 72

T1 Selenomethionyl dihydrofolate reductase from Escherichia coli. Comparative biochemistry and 77Se \*\*\*nuclear\*\*\* \*\*\*magnetic\*\*\* \*\*\*resonance\*\*\* spectroscopy.

L9 ANSWER 160 OF 189 MEDLINE

DUPLICATE 73

T1 Induced \*\*\*peptide\*\*\* conformations in different antibody complexes: molecular modeling of the \*\*\*three\*\*\* - \*\*\*dimensional\*\*\* structure of \*\*\*peptide\*\*\* -antibody complexes using \*\*\*NMR\*\*\* -derived distance restraints.

L9 ANSWER 161 OF 189 MEDLINE

T1 Inhibition of cellular proliferation by \*\*\*peptide\*\*\* analogues of insulin-like growth factor 1.

L9 ANSWER 162 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS DUPLICATE 74

T1 SECONDARY STRUCTURE AND TOPOLOGY OF INTERLEUKIN-1 RECEPTOR ANTAGONIST \*\*\*PROTEIN\*\*\* DETERMINED BY HETERONUCLEAR \*\*\*THREE\*\*\* - \*\*\*DIMENSIONAL\*\*\* \*\*\*NMR\*\*\* SPECTROSCOPY.

L9 ANSWER 163 OF 189 MEDLINE

DUPLICATE 75

T1 Mutations at the dimer, hexamer, and receptor-binding surfaces of insulin independently affect insulin-insulin and insulin-receptor interactions.

L9 ANSWER 164 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS

T1 SOLUTION STUDIES OF STAPHYLOCOCCAL NUCLEASE H124L 2 PROTON CARBON-13 AND NITROGEN-15 CHEMICAL SHIFT ASSIGNMENTS FOR THE UNLIGATED ENZYME AND ANALYSIS OF CHEMICAL SHIFT CHANGES THAT ACCOMPANY FORMATION OF THE NUCLEASE THYMIDINE 3' 5'-BISPHOSPHATE-CALCIUM TERNARY COMPLEX.

L9 ANSWER 165 OF 189 MEDLINE

DUPLICATE 76

T1 Characterization of the bacterially expressed Drosophila engrailed homeodomain.

L9 ANSWER 166 OF 189 EMBASE COPYRIGHT 1999 ELSEVIER SCI. B.V.

T1 RNase H: \*\*\*Three\*\*\* - \*\*\*dimensional\*\*\* \*\*\*structure\*\*\* and \*\*\*function\*\*\*

L9 ANSWER 167 OF 189 MEDLINE

DUPLICATE 77

T1 \*\*\*Structure\*\*\* - \*\*\*function\*\*\* relationships in human epidermal growth factor studied by site-directed mutagenesis and 1H \*\*\*NMR\*\*\*

L9 ANSWER 168 OF 189 MEDLINE

DUPLICATE 78

T1 \*\*\*Structure\*\*\* and \*\*\*structure\*\*\* - \*\*\*function\*\*\* relationships of sea anemone \*\*\*proteins\*\*\* that interact with the sodium channel.

L9 ANSWER 169 OF 189 MEDLINE

T1 \*\*\*Protein\*\*\* crystal growth in microgravity.

L9 ANSWER 170 OF 189 MEDLINE

DUPLICATE 79

T1 Folding and \*\*\*activity\*\*\* of hybrid sequence, disulfide-stabilized \*\*\*peptides\*\*\*

L9 ANSWER 171 OF 189 MEDLINE

DUPLICATE 80

T1 The structure of the homeodomain and its functional implications.

L9 ANSWER 172 OF 189 CAPLUS COPYRIGHT 1999 ACS

T1 Determination of \*\*\*protein\*\*\* structure in aqueous solution with and without distance constraints

L9 ANSWER 173 OF 189 MEDLINE

T1 \*\*\*Proteins\*\*\* as biological effectors.

L9 ANSWER 174 OF 189 MEDLINE DUPLICATE 81  
TI Conformational characterization of a single-site mutant of murine epidermal growth factor (EGF) by 1H \*\*\*NMR\*\*\* provides evidence that leucine-47 is involved in the interactions with the EGF receptor.

L9 ANSWER 175 OF 189 MEDLINE  
TI \*\*\*Three\*\*\* - \*\*\*dimensional\*\*\* \*\*\*structure\*\*\* and \*\*\*function\*\*\* of epidermal growth factor.

L9 ANSWER 176 OF 189 MEDLINE DUPLICATE 82  
TI Enzymatic approaches to probing of RNA secondary and \*\*\*tertiary\*\*\* \*\*\*structure\*\*\*.

L9 ANSWER 177 OF 189 MEDLINE  
TI \*\*\*Tertiary\*\*\* \*\*\*structure\*\*\* of human complement component C5a in solution from \*\*\*nuclear\*\*\* \*\*\*magnetic\*\*\* \*\*\*resonance\*\*\* data.

L9 ANSWER 178 OF 189 LIFESCI COPYRIGHT 1999 CSA  
TI \*\*\*Structure\*\*\* and \*\*\*function\*\*\* of \*\*\*proteins\*\*\*.

L9 ANSWER 179 OF 189 MEDLINE DUPLICATE 83  
TI \*\*\*Structure\*\*\* - \*\*\*function\*\*\* relationship in Escherichia coli translational initiation factors. Characterization of IF1 by high-resolution 1H- \*\*\*NMR\*\*\* spectroscopy.

L9 ANSWER 180 OF 189 MEDLINE DUPLICATE 84  
TI Quaternary \*\*\*structure\*\*\* and \*\*\*function\*\*\* in phage lambda repressor: 1H- \*\*\*NMR\*\*\* studies of genetically altered \*\*\*proteins\*\*\*.

L9 ANSWER 181 OF 189 CAPLUS COPYRIGHT 1999 ACS  
TI Characterization of specific fluorenylmethoxycarbonyl-containing calmodulin adducts by spectroscopy and phosphodiesterase stimulation

L9 ANSWER 182 OF 189 MEDLINE DUPLICATE 85  
TI \*\*\*Structure\*\*\* and \*\*\*function\*\*\* of the proline-rich region of myelin basic \*\*\*protein\*\*\*.

L9 ANSWER 183 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS  
TI ANNUAL REVIEW OF BIOPHYSICS AND BIOENGINEERING VOL. 13 1984.

L9 ANSWER 184 OF 189 MEDLINE DUPLICATE 86  
TI \*\*\*Structure\*\*\* - \*\*\*function\*\*\* relationship in Escherichia coli translational initiation factors. Characterization of IF-3 by high resolution 1H \*\*\*NMR\*\*\* spectroscopy.

L9 ANSWER 185 OF 189 CAPLUS COPYRIGHT 1999 ACS  
TI \*\*\*Structure\*\*\* - \*\*\*function\*\*\* relationship in Escherichia coli initiation factors: VII. Biochemical and proton \*\*\*NMR\*\*\* spectroscopic study on the involvement of the His residue in the interaction between IF3 and ribosomes

L9 ANSWER 186 OF 189 MEDLINE  
TI Physical chemical studies of the \*\*\*structure\*\*\* and \*\*\*function\*\*\* of DNA binding (helix-destabilizing) \*\*\*proteins\*\*\*.

L9 ANSWER 187 OF 189 ENERGY COPYRIGHT 1999 USDOE/IEA-ETDE  
TI Computational tools for experimental determination and theoretical prediction of protein structure.

L9 ANSWER 188 OF 189 ENERGY COPYRIGHT 1999 USDOE/IEA-ETDE  
TI Workshop on high-field NMR and biological applications.

L9 ANSWER 189 OF 189 ENERGY COPYRIGHT 1999 USDOE/IEA-ETDE  
TI Development of experimental techniques to study protein and nucleic acid structures.

=> d 2,17,34,37,40,71,96,106,120,125,147,154,187 bib ab

L9 ANSWER 2 OF 189 CAPLUS COPYRIGHT 1999 ACS  
AN 1999:303259 CAPLUS  
DN 130:308199  
TI Linking gene sequence to gene \*\*\*function\*\*\* by \*\*\*three\*\*\* - \*\*\*dimensional\*\*\* \*\*\*protein\*\*\* \*\*\*structure\*\*\* determination using \*\*\*NMR\*\*\*  
IN Anderson, Stephen; Montelione, Gaetano  
PA Rutgers, the State University of New Jersey, USA  
SO PCT Int. Appl., 56 pp.  
CODEN: PIXXD2  
DT Patent  
LA English  
FAN.CNT 1  
PATENT NO. KIND DATE APPLICATION NO. DATE

PI WO 9922019 A1 19990506 WO 1998-US22839 19981029  
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE,

KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRAI US 1997-63679 19971029

US 1998-181601 19981029

AB The present invention provides a \*\*\*structure\*\*\* - \*\*\*functional\*\*\* anal. engine for the high-throughput detn. of the biochem. \*\*\*function\*\*\* of \*\*\*proteins\*\*\* or \*\*\*protein\*\*\* domains of unknown \*\*\*function\*\*\*. The present invention uses bioinformatics, mol. biol. and \*\*\*NMR\*\*\* tools for the rapid and automated detn. of the \*\*\*three\*\*\* - \*\*\*dimensional\*\*\* structures of \*\*\*proteins\*\*\* and \*\*\*protein\*\*\* domains.

L9 ANSWER 17 OF 189 CAPLUS COPYRIGHT 1999 ACS

AN 1999:146268 CAPLUS

TI \*\*\*Protein\*\*\* \*\*\*NMR\*\*\* and the human proteome project

AU Montelione, Gaetano T.

CS Center for Advanced Biotechnology Medicine and Department of Molecular Biology and Biochemistry, Rutgers University, Piscataway, NJ, 08854, USA

SO Book of Abstracts, 217th ACS National Meeting, Anaheim, Calif., March 21-25 (1999), POLY-232 Publisher: American Chemical Society, Washington, D. C.

CODEN: 67GHA6

DT Conference; Meeting Abstract

LA English

AB Genome sequencing projects are rapidly identifying all of the genes in several organisms. The products of these genes are widely recognized as the next generation of therapeutics and targets for the development of pharmaceuticals. While identification of these genes is proceeding quickly, elucidation of their \*\*\*three\*\*\* - \*\*\*dimensional\*\*\* (3D) \*\*\*structures\*\*\* and biochem. \*\*\*functions\*\*\* lags far behind. In some cases, knowledge of 3D structures of \*\*\*proteins\*\*\* can provide important insights into structural homol. that is not easily recognized by sequence alignment comparisons. Thus, anal. of a \*\*\*protein\*\*\* 's 3D structure by \*\*\*NMR\*\*\* or X-ray crystallog. prior to characterization of the \*\*\*protein\*\*\* 's biochem. \*\*\*function\*\*\* can sometimes provide key information regarding \*\*\*protein\*\*\* fold class, locations and clustering of conserved residues, and surface electrostatic field distributions. This information can be used to develop hypotheses regarding potential biochem. functions, and the resulting limited set of putative biochem. functions tested by appropriate biochem. assays. \*\*\*NMR\*\*\* chem. shift assignments and soln. structures of \*\*\*proteins\*\*\* also provide the basis for epitope-mapping, mol. dynamics, and SAR studies, and set the stage for subsequent drug development using combinatorial and/or rational design methods. We are developing technologies that will significantly accelerate the process of structure detn. by \*\*\*NMR\*\*\*. These include bioinformatics methods for parsing novel genes into domain encoding regions, high-level "multiplexed" \*\*\*protein\*\*\* expression systems, and \*\*\*NMR\*\*\* pulse sequences, data collection methods, and expert-system software for automated anal. of \*\*\*protein\*\*\* resonance assignments and 3D structures. These technologies and the resulting expl. data are being organized and integrated using relational databases. The goal of this work is to develop a "high-throughput" process for structural anal. of novel gene products on a genomic scale. In a pilot project, these techniques are being applied to clusters of orthologous genes coding for \*\*\*proteins\*\*\* of unknown \*\*\*structure\*\*\* and \*\*\*function\*\*\*, with the aim of testing the hypothesis that 3D structural anal. can sometimes provide useful and important clues regarding the biochem. functions of orphan gene products. The relationship of our effort and the emerging international interest in a large-scale Human Proteome Project will be discussed.

L9 ANSWER 34 OF 189 MEDLINE DUPLICATE 17  
AN 199837899 MEDLINE

DN 98387899

TI Method for prediction of \*\*\*protein\*\*\* \*\*\*function\*\*\* from sequence using the sequence-to- \*\*\*structure\*\*\* -to- \*\*\*function\*\*\* paradigm with application to glutaredoxins/thioredoxins and T1 ribonucleases.

AU Fetrow J S; Skolnick J

CS Center for Biochemistry and Biophysics, University at Albany, SUNY, 1400 Washington Avenue, Albany, NY 12222, USA.

SO JOURNAL OF MOLECULAR BIOLOGY, (1998 Sep 4) 281 (5) 949-68. Journal code: J6V. ISSN: 0022-2836.

CY ENGLAND: United Kingdom

DT Journal; Article; (JOURNAL ARTICLE)

LA English

FS Priority Journals; Cancer Journals

EM 199812

EW 19981202

AB The practical exploitation of the vast numbers of sequences in the genome sequence databases is crucially dependent on the ability to identify the \*\*\*function\*\*\* of each sequence. Unfortunately, current methods, including global sequence alignment and local sequence motif identification, are limited by the extent of sequence similarity between sequences of unknown and known \*\*\*function\*\*\*; these methods

increasingly fail as the sequence identity diverges into and beyond the twilight zone of sequence identity. To address this problem, a novel method for identification of \*\*\*protein\*\*\* \*\*\*function\*\*\* based directly on the sequence-to-\*\*\*structure\*\*\* -to- \*\*\*function\*\*\* paradigm is described. Descriptors of \*\*\*protein\*\*\* active sites, termed "fuzzy functional forms" or FFFs, are created based on the geometry and conformation of the active site. By way of illustration, the active sites responsible for the disulfide oxidoreductase \*\*\*activity\*\*\* of the glutaredoxin/thioredoxin family and the RNA hydrolytic \*\*\*activity\*\*\* of the T1 ribonuclease family are presented. First, the FFFs are shown to correctly identify their corresponding active sites in a library of exact \*\*\*protein\*\*\* models produced by crystallography or \*\*\*NMR\*\*\* spectroscopy, most of which lack the specified \*\*\*activity\*\*\*. Next, these FFFs are used to screen for active sites in low-to-moderate resolution models produced by ab initio folding or threading prediction algorithms. Again, the FFFs can specifically identify the functional sites of these \*\*\*proteins\*\*\* from their predicted structures. The results demonstrate that low-to-moderate resolution models as produced by state-of-the-art \*\*\*tertiary\*\*\* \*\*\*structure\*\*\* prediction algorithms are sufficient to identify \*\*\*protein\*\*\* active sites. Prediction of a novel \*\*\*function\*\*\* for the gamma subunit of a yeast glycosyl transferase and prediction of the \*\*\*function\*\*\* of two hypothetical yeast \*\*\*proteins\*\*\* whose models were produced via threading are presented. This work suggests a means for the large-scale functional screening of genomic sequence databases based on the prediction of structure from sequence, then on the identification of functional active sites in the predicted structure. Copyright 1998 Academic Press

L9 ANSWER 37 OF 189 MEDLINE  
AN 1998290966 MEDLINE  
DN 98290966  
TI Recent trends in \*\*\*protein\*\*\* structural studies.  
AU Titani K; Hayashi N  
CS Division of Biomedical Polymer Science, Institute for Comprehensive Medical Science, Fujita Health University, Toyoake  
SO RINSHO BYORI. JAPANESE JOURNAL OF CLINICAL PATHOLOGY, (1998 May) 46 (5)  
450-5. Ref: 0  
Journal code: KIV. ISSN: 0047-1860.

CY Japan  
DT Journal; Article; (JOURNAL ARTICLE)  
General Review; (REVIEW)  
(REVIEW LITERATURE)

LA Japanese  
EM 199810  
EW 19981005

AB Since the 1980's, structural studies of \*\*\*proteins\*\*\* have changed remarkably. It is currently possible to predict the entire amino acid sequence of a \*\*\*protein\*\*\* by the rapid and highly sensitive analysis of the nucleotide sequence of genomic DNA or cDNA encoding the \*\*\*protein\*\*\*. In the near future, the entire sequence of a \*\*\*protein\*\*\* may be predicted from a partial sequence just by searching a variety of databases now being constructed for many biological species. The predicted \*\*\*protein\*\*\* sequence, however, is the backbone structure of the precursor \*\*\*protein\*\*\* without post-translational modifications. Therefore, the major objectives of recent structural studies of \*\*\*proteins\*\*\* are directed to 1) rapid and sensitive confirmation of the predicted sequence and identification of those modifications present in mature \*\*\*proteins\*\*\* by newly developed mass spectrometry, 2) determination of the 3D structures of intact and mutant \*\*\*proteins\*\*\* isolated or expressed in cultured E. coli, yeast or animal cells using X-ray crystallography or \*\*\*NMR\*\*\* analysis, and 3) rapid prediction of the 3D structures of \*\*\*proteins\*\*\* utilizing \*\*\*protein\*\*\* databases. The "PROTEOME" project was proposed in 1998 to bring together all the data on the \*\*\*structure\*\*\* and \*\*\*function\*\*\* of mature \*\*\*proteins\*\*\* under international cooperation. The present paper summarizes such recent trends in \*\*\*protein\*\*\* structural studies.

L9 ANSWER 40 OF 189 CAPLUS COPYRIGHT 1999 ACS  
AN 1998.328663 CAPLUS  
DN 129:133145  
TI The development of \*\*\*NMR\*\*\* methods to study \*\*\*protein\*\*\* structure and dynamics  
AU Kay, Lewis E.  
CS Departments of Medical Genetics, Biochemistry and Chemistry, University of Toronto, Toronto, ON, M5S 1A8, Can.  
SO NATO ASI Ser., Ser. C (1998), 510(New Methods for the Study of Biomolecular Complexes), 285-293  
CODEN: NSCSDW, ISSN: 0258-2023  
PB Kluwer Academic Publishers  
DT Journal; General Review  
LA English  
AB A review with 28 refs. An understanding of the role played by a \*\*\*protein\*\*\* in cellular \*\*\*function\*\*\* requires a detailed picture of its \*\*\*three\*\*\* - \*\*\*dimensional\*\*\* structure as well as an appreciation of how the \*\*\*structure\*\*\* varies as a \*\*\*function\*\*\* of time due to mol. dynamics. Over the past several years multi-dimensional, multi-nuclear soln. \*\*\*NMR\*\*\* spectroscopy has become a powerful technol. for obtaining both structural and dynamic

information on \*\*\*proteins\*\*\* and \*\*\*protein\*\*\* -ligand systems. However, until recently the methods were limited to the study of mols. having mol. wts. on the order of 25 kDa or less. Recent developments making use of fractional or complete deuteration have increased the scope of structural studies by \*\*\*NMR\*\*\* and have also improved studies of

L9 ANSWER 71 OF 189 MEDLINE  
AN 1998046743 MEDLINE  
DN 98046743  
TI TESS: a geometric hashing algorithm for deriving 3D coordinate templates for searching structural databases. Application to enzyme active sites.  
AU Wallace A C; Borkakoti N; Thornton J M  
CS Department of Biochemistry and Molecular Biology, University College, London, England.  
SO PROTEIN SCIENCE, (1997 Nov) 6 (11) 2308-23.  
Journal code: BNW. ISSN: 0961-8368.  
EM 199804  
EW 19980403

AB It is well established that sequence templates such as those in the PROSITE and PRINTS databases are powerful tools for predicting the biological \*\*\*function\*\*\* and \*\*\*tertiary\*\*\* \*\*\*structure\*\*\* for newly derived \*\*\*protein\*\*\* sequences. The number of X-ray and \*\*\*NMR\*\*\* \*\*\*protein\*\*\* structures is increasing rapidly and it is apparent that a 3D equivalent of the sequence templates is needed. Here, we describe an algorithm called TESS that automatically derives 3D templates from structures deposited in the Brookhaven \*\*\*Protein\*\*\* Data Bank. While a new sequence can be searched for sequence patterns, a new structure can be scanned against these 3D templates to identify functional sites. As examples, 3D templates are derived for enzymes with an O-His-O "catalytic triad" and for the ribonucleases and lysozymes. When these 3D templates are applied to a large data set of nonidentical \*\*\*proteins\*\*\*, several interesting hits are located. This suggests that the development of a 3D template database may help to identify the \*\*\*function\*\*\* of new \*\*\*protein\*\*\* \*\*\*structures\*\*\*, if unknown, as well as to design \*\*\*proteins\*\*\* with specific functions.

L9 ANSWER 96 OF 189 MEDLINE  
AN 97120677 MEDLINE  
DN 97120677  
TI What \*\*\*function\*\*\* for human lithostathine?: structural investigations by \*\*\*three\*\*\* - \*\*\*dimensional\*\*\* structure modeling and high-resolution \*\*\*NMR\*\*\* spectroscopy.  
AU Patard L; Stoven V; Gharib B; Bontems F; Lallemand J Y; De Reggi M  
CS Laboratoire de RMN, URA 1308 du CNRS, DCSO, Ecole Polytechnique, Palaiseau, France.  
SO PROTEIN ENGINEERING, (1996 Nov) 9 (11) 949-57.  
Journal code: PRI. ISSN: 0269-2139.  
CY ENGLAND: United Kingdom  
DT Journal; Article; (JOURNAL ARTICLE)  
LA English  
FS Priority Journals  
EM 199705  
EW 19970504

AB Human lithostathine is a 144-residue \*\*\*protein\*\*\*, expressed in various organs and pathologies. Several biological functions have been proposed for this \*\*\*protein\*\*\*. Among others, inhibition of nucleation and growth of CaCO<sub>3</sub> crystals in the pancreas and bacterial aggregation has retained attention, because lithostathine presents high sequence similarities with calcium-dependent (or C-type) lectins. To study its \*\*\*structure\*\*\* - \*\*\*function\*\*\* relationship and compare it with that of C-type lectins, we have built a model for lithostathine. This model is derived from the only two C-type lectins of known structures: rat mannose binding \*\*\*protein\*\*\* and human E-selectin. An original strategy, inspired by that proposed by Havel and Snow, was designed for model building. We have undertaken \*\*\*NMR\*\*\* studies on the natural \*\*\*protein\*\*\*. Although complete structure determination has not yet been achieved, the \*\*\*NMR\*\*\* studies did confirm the main characteristics of the model. From analysis of the proposed model, we concluded that lithostathine is not expected to present sugar- or calcium-binding properties. Therefore, the mechanisms of bacterial aggregation and inhibition of CaCO<sub>3</sub> nucleation and growth have not yet been elucidated.

L9 ANSWER 106 OF 189 CAPLUS COPYRIGHT 1999 ACS  
AN 1996.202695 CAPLUS  
DN 124:253414  
TI Modern \*\*\*NMR\*\*\* spectroscopy and x-ray crystallography. Different approaches to study the \*\*\*structure\*\*\* and its \*\*\*function\*\*\* of a \*\*\*protein\*\*\*  
AU Tsuda, Sakae  
CS Biosci. Chem. Div., Hokkaido Natl. Ind. Res. Inst., Sapporo, 062, Japan  
SO Nippon Kessho Gakkaishi (1996), 38(1), 84-8  
CODEN: NKEGAF; ISSN: 0369-4585  
DT Journal; General Review  
LA Japanese  
AB A review with 27 refs. The \*\*\*NMR\*\*\* spectroscopy has been utilized widely for an elucidation of the structural changes of \*\*\*proteins\*\*\* caused by changes in pH, ionic strength, temp., and ligand concn. in soln. The x-ray was less utilized for these studies executable easily in soln., but is utilized much for the structural detn. of a \*\*\*protein\*\*\*.

Such difference has lead to the situation where the \*\*\*NMR\*\*\* relied on the structure solved by x-ray and the x-ray argued its structure in ref. to the conformational change elucidated by \*\*\*NMR\*\*\*. However, recent developments of \*\*\*NMR\*\*\* spectroscopy made it possible to det. the \*\*\*three\*\*\* - \*\*\*dimensional\*\*\* structure, and x-ray techniques has also been developed to clarify the structural changes of a \*\*\*protein\*\*\*. This review compares the recent development of these two techniques, and will discuss about the future collaborating interaction between \*\*\*NMR\*\*\* and x-ray.

L9 ANSWER 120 OF 189 BIOSIS COPYRIGHT 1999 BIOSIS

AN 1995:309145 BIOSIS

DN PREV199598323445

TI \*\*\*NMR\*\*\* : This other method for \*\*\*protein\*\*\* and nucleic acid structure determination.

AU Wuthrich, Kurt

CS Inst. Molekularbiol. und Biophysik, Eidgenossische Technische Hochschule-Honggerberg, CH-8093 Zurich Switzerland

SO Acta Crystallographica Section D Biological Crystallography, (1995) Vol. 51, No. 3, pp. 249-270.  
ISSN: 0907-4449.

AB For a quarter of a century X-ray diffraction in single crystals was unique in its ability to solve \*\*\*three\*\*\* - \*\*\*dimensional\*\*\* structures of \*\*\*proteins\*\*\* and nucleic acids at atomic resolution. The situation changed in 1984 with the completion of a \*\*\*protein\*\*\* structure determination by \*\*\*nuclear\*\*\* \*\*\*magnetic\*\*\* \*\*\*resonance\*\*\* (\*\*\*NMR\*\*\* ) spectroscopy in solution, and today \*\*\*NMR\*\*\* is a second widely used method for biomacromolecular structure determination. This review describes the method of \*\*\*NMR\*\*\* structure determination of biological macromolecules, and attempts to place \*\*\*NMR\*\*\* structure determination in perspective with X-ray crystallography. \*\*\*NMR\*\*\* is most powerful for studies of relatively small systems with molecular weights up to about 30000, but these structures can be obtained in near-physiological milieus. The two techniques have widely different time scales which afford different insights into internal molecular mobility as well as different views of \*\*\*protein\*\*\* or nucleic acid molecular surfaces and hydration. Generally, in addition to information on the average \*\*\*three\*\*\* - \*\*\*dimensional\*\*\* structure, \*\*\*NMR\*\*\* provides information on a wide array of short-lived transient conformational states. Combining information from the two methods can yield a more detailed insight into the structural basis of \*\*\*protein\*\*\* and nucleic acid functions, and thus provide a more reliable platform for rational drug design and the engineering of novel \*\*\*protein\*\*\* functions.

L9 ANSWER 125 OF 189 CAPLUS COPYRIGHT 1999 ACS DUPLICATE 62

AN 1995:774534 CAPLUS

DN 123:163615

TI \*\*\*Structure\*\*\* and \*\*\*function\*\*\* of \*\*\*protein\*\*\* modules

AU Go, Mitiko

CS Toyota Phys. Chem. Res. Inst., Aichi, 480-11, Japan

SO Toyota Kenkyu Hokoku (1995), 48, 81-5

CODEN: TOKHA6; ISSN: 0372-039X

LA Japanese

AB Globular \*\*\*proteins\*\*\* are decompd. into several compact modules. Modules consist of about 10-40 contiguous amino acid residues and module boundaries are correlated with intron positions of genes. To clarify physico-chem. basis of modules as structural units of \*\*\*proteins\*\*\*, the authors synthesized module M1 of barnase, a bacterial RNase, and detd. its secondary structure in soln. by using \*\*\*NMR\*\*\* technique. M1 had an .alpha.-helix at the similar location to the corresponding helix of the intact barnase. This result shows that the excised module has propensity to form similar secondary structure to those of the intact barnase. This propensity should be an important feature of modules advantageous as parts recruited into globular \*\*\*proteins\*\*\* through exon shuffling in early evolution. To identify functionally important regions of large \*\*\*proteins\*\*\* without their \*\*\*three\*\*\* - \*\*\*dimensional\*\*\* information, the authors applied a method for prediction of module boundaries to human CCG1. The authors obtained a close correlation between predicted modules and exon/intron structure of human CCG1 gene. Predicted 152 modules of CCG1 show a close correlation with temporary assigned \*\*\*function\*\*\* of CCG1. This result opens a new exptl. approach to det. functionally important regions of huge \*\*\*proteins\*\*\*; synthesis of a module or jointed modules of the \*\*\*proteins\*\*\* by chem. method and detn. of its \*\*\*function\*\*\* will be useful for identification of each functional region of \*\*\*proteins\*\*\*.

L9 ANSWER 147 OF 189 CAPLUS COPYRIGHT 1999 ACS

AN 1995:473516 CAPLUS

DN 122:234586

TI \*\*\*Function\*\*\* and \*\*\*three\*\*\* - \*\*\*dimensional\*\*\* \*\*\*structure\*\*\* of \*\*\*proteins\*\*\* using \*\*\*nuclear\*\*\* \*\*\*magnetic\*\*\* \*\*\*resonance\*\*\* spectroscopy

AU Poulsen, Flemming M.

CS Kemisk Afdeling, Carlsberg Laboratorium, Copenhagen, DK-2500, Den.

SO Protein Struct. Distance Anal. (1994), 24-35, 2 plate. Editor(s): Bohr, Henrik; Brunak, Soeren. Publisher: IOS Press, Amsterdam, Neth.

CODEN: 61CIAF

DT Conference

LA English

AB Although the \*\*\*three\*\*\* - \*\*\*dimensional\*\*\* structure of a \*\*\*protein\*\*\* can provide valuable information and stimulate rational investigation of other important features of the \*\*\*protein\*\*\* it is important to stress that a structure per se is rarely a revelation of the biol. \*\*\*function\*\*\* of the \*\*\*protein\*\*\*. This paper emphasizes the importance of acquiring results that measure the fundamental phys. chem. parameters in \*\*\*protein\*\*\* \*\*\*function\*\*\* events and the importance of getting quant. information to support our understanding of the link between phys. parameters that describe \*\*\*function\*\*\* and the biol. relevance of a \*\*\*protein\*\*\* mol. It is emphasized that \*\*\*NMR\*\*\* spectroscopy, because it combines the ability of measuring \*\*\*three\*\*\* - \*\*\*dimensional\*\*\* structure and the ability of measuring many phys. parameters related to both \*\*\*structure\*\*\* and \*\*\*function\*\*\*, is one of the key techniques in structural biol.

L9 ANSWER 154 OF 189 MEDLINE

DUPLICATE 71

AN 93184745 MEDLINE

DN 93184745

TI An automated method for modeling \*\*\*proteins\*\*\* on known templates using distance geometry.

AU Srinivasan S; March C J; Sudarsanam S

CS Department of Protein Chemistry, Immunex Corporation, Seattle, Washington 98101..

SO PROTEIN SCIENCE, (1993 Feb) 2 (2) 277-89.

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AB We present an automated method incorporated into a software package, FOLDER, to fold a \*\*\*protein\*\*\* sequence on a given \*\*\*three\*\*\* - \*\*\*dimensional\*\*\* (3D) template. Starting with the sequence alignment of a family of homologous \*\*\*proteins\*\*\*, tertiary structures are modeled using the known 3D structure of one member of the family as a template. Homologous interatomic distances from the template are used as constraints. For nonhomologous regions in the model \*\*\*protein\*\*\*, the lower and the upper bounds for the interatomic distances are imposed by steric constraints and the globular dimensions of the template, respectively. Distance geometry is used to embed an ensemble of structures consistent with these distance bounds. Structures are selected from this ensemble based on minimal distance error criteria, after a penalty \*\*\*function\*\*\* optimization step. These \*\*\*structures\*\*\* are then refined using energy optimization methods. The method is tested by simulating the alpha-chain of horse hemoglobin using the alpha-chain of human hemoglobin as the template and by comparing the generated models with the crystal structure of the alpha-chain of horse hemoglobin. We also test the packing efficiency of this method by reconstructing the atomic positions of the interior side chains beyond C beta atoms of a \*\*\*protein\*\*\* domain from a known 3D structure. In both test cases, models retain the template constraints and any additionally imposed constraints while the packing of the interior residues is optimized with no short contacts or bond deformations. To demonstrate the use of this method in simulating structures of \*\*\*proteins\*\*\* with nonhomologous disulfides, we construct a model of murine interleukin (IL)-4 using the \*\*\*NMR\*\*\* structure of human IL-4 as the template. The resulting geometry of the nonhomologous disulfide in the model structure for murine IL-4 is consistent with standard disulfide geometry.

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TI Computational tools for experimental determination and theoretical prediction of protein structure.

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AB This tutorial was one of eight tutorials selected to be presented at the Third International Conference on Intelligent Systems for Molecular Biology which was held in the United Kingdom from July 16 to 19, 1995. The authors intend to review the state of the art in the experimental determination of protein 3D structure (focus on nuclear magnetic resonance), and in the theoretical prediction of protein function and of protein structure in 1D, 2D and 3D from sequence. All the atomic resolution structures determined so far have been derived from either X-ray crystallography (the majority so far) or Nuclear Magnetic Resonance (NMR) Spectroscopy (becoming increasingly more important). The authors briefly describe the physical methods behind both of these techniques; the major computational methods involved will be covered in some detail. They highlight parallels and differences between the methods, and also the current limitations. Special emphasis will be given to techniques which have application to ab initio structure prediction. Large scale sequencing techniques increase the gap between the number of known proteins sequences and that of known protein structures. They describe the scope and principles of methods that contribute successfully to closing that gap. Emphasis will be given on the specification of adequate testing procedures to validate such methods